

# Semi-classical, microscopic approach to the liquid drop model - a possible way of the description of heavy ion reaction.

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April 11, 2013

## Abstract

An isospin and spin dependent form of the equation of state for nuclear matter is presented. This form is used for the description of nucleon interaction in a new dynamic model. Preliminary calculations show that the new approach makes possible predicting the alpha structures appearing in the case of the ground state even-even nuclei. The change in the structure of nuclei built on the basis of alpha particles occurring for  $^{60}\text{Zn}$  is discussed.

## 1 Introduction

Although nuclei are close to 55 orders of magnitude lighter than a typical neutron star, it seems that the state of the material comprising of the above two objects can be determined by the same equation, which is the equation of state (EOS) of nuclear matter. In this case EOS is defined as the average energy per baryon expressed as a function of thermodynamic variables. It would seem that the above statement can be more easily justified for heavy nuclei but, as can be shown, using an appropriate form of the equation of state can give good results also for the description of the ground states for lighter nuclei. We arrive at these conclusions using semiclassical, microscopic version of the liquid drop model in which dynamics is governed by EOS.

The description of dynamics of nuclear system, which uses the concept of the equation of state, can

be found in the reaction models referring to the liquid drop model (LDM) [1]. In this description, it is assumed that the energy of the system is determined mainly by using the following three components:

- the volume energy defined by the kinetic energy related to internal, fermionic motion and respective potential interactions for infinite nuclear matter in equilibrium,
- the surface energy, which in classical description could be treated as a result of the surface tension action,
- the Coulomb energy associated with the proton charge.

Such models typically assume one body dissipation and no compression of the nuclear matter. In such an approach the volume energy together with energies which are corrections related to a not equal number of protons and neutrons and a non-zero spin of the system may be treated as the  $0^{th}$  term of the expansion of the energy density function (given by EOS). No matter compression assumed in this model introduces additional constraints on the global coordinates which describe the system shape and its evolution.

In our microscopic description of the system evolution, we take into account also the next term of the expansion of the equation of state as a function of the density of nuclear matter. The presented approach treats the local density of nuclear matter as a result of the aggregation of partial densities given by Gaussian packets which represent the nucleons forming the system. As a result, the local density of matter is explicitly given by the position of these packages

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and their variance. In our approach we describe the volume energy as the respective functional (volume integral of the energy density given by the equation of state multiplied by the density of the nuclear matter).

The nuclear EOS describes equilibrated, infinite nuclear matter and is necessary to calculate the properties of astronomical objects as, for example, neutron stars or supernovae [2]. In such large objects, the surface effect in the description of the total energy is negligible. For small objects, such as atomic nuclei, the energy due to interactions at the surface, cannot be ignored and in such case the Hamiltonian values must have additional contributions, corresponding to this additional surface energy. In the presented approach, the surface energy is related to the dispersion of the energy density in the nucleon's environment and also to the increase of the diffuseness of the nucleon momentum caused by nucleon location on the surface (reduce the uncertainty given by surface interactions as described in [3]).

In the interaction description which is applied in the model presented here one can distinguish ingredients related to the volume, surface and Coulomb energy, which are the essence of description used in LDM model.

In our approach, all the aforementioned types of energy are functionals expressed by integrals determined by the distribution of nuclear matter. Since these densities are here uniquely determined by the position and other parameters of wave packets (spin, isospin and variance), the description can be interpreted as the Microscopic LDM model (MLDM).

As we know, the equation of state of nuclear matter is still not well established and its determination is one of the most important tasks faced by experimental and theoretical nuclear physics. In the presented approach, the equation of state plays a very important role and in this way the described model has an opportunity to contribute in EOS investigation. It is also important to use a convenient form of EOS suitable for efficient description of the heavy ion reaction as well as for description of the ground state properties of the reacted nuclei. This form of EOS should fulfill the following requirements:

1. The compression part of the equation of state,

in the neighborhood of saturation density  $\rho_0$  (where  $\rho_0$  is the density of the matter which is equilibrated in isospin and spin and for which the density of energy reaches a minimum) can be written as the sum of the two types of energy:

- $e_0$ : energy related to symmetric nuclear matter SNM;
- $e_{sym}$ : energy produced by the nuclear matter symmetry disorders, which is called symmetry energy (see section 2).

It turns out that by the adoption of certain simplifying assumptions (see appendix A), these energies can be expressed as a function of the total density of  $\rho$ . The expectation which is in line with a mean field theory (e.g. with the Skyrme-Hartree-Fock model) determine the zero energy density in case where density of matter tends to zero (it is in contrast with some other models like, for instance, an idealized alpha-matter picture [4]).

2. For the saturation density we require:

- specific value of the energy density;
- specific values of the first and the second derivative of the energy density (defined by EOS);
- and for density  $\rho \rightarrow 0$  the additional requirement is  $e(\rho) \rightarrow 0$

then the simplest form of a polynomial, which can meet all these requirements can be expressed as:

$$e = \alpha\rho + \beta\rho^2 + \gamma\rho^3 \quad (1)$$

The method of determining the coefficients alpha, beta, gamma is given in Section 2. and Appendix A. As it is shown [3], form (1) is suitable for different theoretical descriptions of EOS. It is also worth noting that this form of the EOS allows us to find the respective mean energy values in an analytical way (in case when the density is expressed by partial density, taken as the Gaussian functions).

A modified equation of state in a form suitable for MLDM calculations is defined in the next section. In the third section we will present the application of the proposed form of the EOS together with an additional surface energy term used in MLDM model. The obtained preliminary results using this model are related to the properties of nuclei in its ground states and are presented in Section 4. Since in our descrip-

tion we use EOS, in which energy symmetry is associated with spin and isospin asymmetry (see next section), the geometric structure defined by the position of the centers of the wave packets can be interpreted as clusters. For the nuclei with even and equal number of neutrons and protons these clusters appear as alpha particles. In Section 5 we present such alpha structures, which appear in model calculations for light nuclei.

In the last chapter conclusions and future plans are presented.

## 2 An equation of state given by third-degree polynomials

The concept of the equation of state of nuclear matter in the case of two-component proton-neutron gas has been discussed in many articles. This equation as well as a form based on the use of the description of third-degree polynomials is described in [3] and works cited therein. In the next section we present the ground state properties of nuclei which are obtained by the microscopic, density-functional approach. EOS plays a key role in this approach.

This model is designed to explore the dependence of the dynamics on wave packets, isospin and the spin of nucleons, which these packets represent. By isospin dependence, we mean the dependence on the charge of the nucleon (third component of isospin vector).

If the isospins, spins and variances of wave packets are the variables affecting the mutual interaction of nucleons, then appropriate equations of state must describe a gas consisting of four components:

- protons with spin up - density  $\rho_{p\uparrow}$
- protons with spin down - density  $\rho_{p\downarrow}$
- neutron with spin up - density  $\rho_{n\uparrow}$
- neutron with spin down, density  $\rho_{n\downarrow}$

In our considerations, by 'nucleons with spin up' or 'nucleons with spin down' we mean nucleons having spin projections 'up' or 'down' on the chosen quantization axis. Now the EOS can be formally written:

$$e = e(\rho_{p\uparrow}, \rho_{p\downarrow}, \rho_{n\uparrow}, \rho_{n\downarrow}) \quad (2)$$

According to symmetries characterizing the nuclear interaction, the system energy is conserved during mutual exchange of neutrons and protons, and also when changing the projection of the spin of all particles to the opposite spin. To allow us to use these symmetries we define new coordinates:

$$\xi = \frac{\rho - \rho_0}{\rho_0} \quad (3)$$

$$\delta = \frac{\rho_n - \rho_p}{\rho} \quad (4)$$

$$\eta_n = \frac{\rho_{n\uparrow} - \rho_{n\downarrow}}{\rho} \quad (5)$$

$$\eta_p = \frac{\rho_{p\uparrow} - \rho_{p\downarrow}}{\rho} \quad (6)$$

where  $\rho$  is the total nuclear matter density, and  $\rho_0$  is the density of isospin and spin balanced matter at saturation. We find that during the above-mentioned operation (mutual conversion of neutrons into protons and the change all the nucleon spin projections) the sign of the coordinates: neutron-proton asymmetry  $\delta$  and spin asymmetry  $\eta_n$  and  $\eta_p$  are respectively changed. Therefore in order to assure energy conservation, in the expression which defines the system energy the values  $\delta$  and  $\eta_n$  and  $\eta_p$  can occur only as products with the respective even number of factors. Using these symmetries one can show (see Appendix A) that the equation of state can be written with the components having an extended form of symmetry energy:

$$\begin{aligned} e = e_{00} &+ \frac{K_0}{18}\xi^2 + \\ &\delta^2 \left( e_{I0} + \frac{L_I}{3}\xi + \frac{K_I}{18}\xi^2 \right) + \\ &(\eta_n^2 + \eta_p^2) \left( e_{ii0} + \frac{L_{ii}}{3}\xi + \frac{K_{ii}}{18}\xi^2 \right) + \\ &2\eta_n\eta_p \left( e_{ij0} + \frac{L_{ij}}{3}\xi + \frac{K_{ij}}{18}\xi^2 \right) \end{aligned} \quad (7)$$

The first two components of the sum (7) represent a well-known form of the equation of state. The first component describes the matter in a balanced system

(zero isospin and spin), where  $K_0$  is the coefficient of compressibility of nuclear matter and the second one describes the isospin interaction is given in the following form:

$$e_I = e_{I0} + \frac{L_I}{3}\xi + \frac{K_I}{18}\xi^2 \quad (8)$$

which is called the symmetry energy for which  $e_{I0}$  is the Wigner constant and the coefficients  $L_I$  and  $K_I$  are the slope and curvature respectively.

In equation (7), by analogy to the isospin symmetry energy, one can distinguish the spin symmetry energies for the neutrons and protons separately:

$$e_{ii} = e_{ii0} + \frac{L_{ii}}{3}\xi + \frac{K_{ii}}{18}\xi^2 \quad (9)$$

and energy:

$$e_{ij} = e_{ij0} + \frac{L_{ij}}{3}\xi + \frac{K_{ij}}{18}\xi^2 \quad (10)$$

for the mutual, spin interaction of protons and neutrons. Factors develop spin symmetry energy:  $e_{ii0}$ ,  $L_{ii}$  and  $K_{ii}$ , (constant slope and curvature) with indices  $ii$ , describe the energy relating to the proton or neutron gas. While the respective indices  $ij$  indicate that the symmetry energy refers to the mutual interaction of protons and neutrons.

All types of the symmetry energy describe the impact of the spin and isospin polarization of the matter on the average energy of the nucleon (EOS). According to the observations presented in the introduction of work, we assume that the energy associated with the SNM as well as all types of symmetry energy should disappear as the density of matter tends to zero. Therefore, to ensure zero values for all energies occurring in equation (7) at  $\rho = 0$  and to get the proper slope and curvature of the saturation density  $\rho_0$  we use the form of third-degree polynomial proposed in [3]. As mentioned in the cited work, if the density of matter is described by the sum of Gaussian distributions, then such a form of the EOS allows us to calculate the average energy analytically.

Any type of energy found in (7) may be written as:

$$e_k = \alpha_k \rho + \beta_k \rho^2 + \gamma_k \rho^3 \quad (11)$$

and the index ' $k$ ' can take values 0,  $I$ ,  $ii$ , and  $ij$ . Here the coefficients  $\alpha_k$ ,  $\beta_k$ ,  $\gamma_k$  are determined by the relations:

$$\alpha_k = \left(3e_{k0} - \frac{2}{3}L_k + \frac{K_k}{18}\right) / \rho_0 \quad (12)$$

$$\beta_k = -\left(3e_{k0} - L_k + \frac{K_k}{9}\right) / \rho_0^2 \quad (13)$$

$$\gamma_k = \left(e_{k0} - \frac{L_k}{3} + \frac{K_k}{18}\right) / \rho_0^3 \quad (14)$$

### 3 Application of the proposed EOS form to the MLDM calculations

The proposed MLDM model, similarly like in [9],[10],[11], describes the time evolution of the wave function represented by the product of  $M$  Gaussian wave packets, which represent the nucleons forming the system :

$$\Phi = \prod_{k=1}^M \phi_k \quad (15)$$

$$\phi_k = \frac{1}{(2\pi\sigma_k^2)^{3/4}} \exp\left(\frac{-(\mathbf{r} - \langle\mathbf{r}_k\rangle)^2}{4\sigma_k^2} + \frac{i}{\hbar}\mathbf{r} \cdot \langle\mathbf{p}_k\rangle\right) \quad (16)$$

where  $\sigma_k^2$ ,  $\langle\mathbf{r}_k\rangle$ ,  $\langle\mathbf{p}_k\rangle$ , are the width of a Gaussian wave function and the centers of its position and associated momentum for each of  $M$  nucleons. In our approach the variables  $\langle\mathbf{r}_k\rangle$ ,  $\langle\mathbf{p}_k\rangle$  and  $\sigma_k^2$  are time-dependent parameters describing the wave functions. Additionally, we assume that with every wave packet for each of  $M$  nucleons, isospin and spin are associated and that they remain fixed during the interaction.

The equations of motion of variables  $\langle\mathbf{r}_k\rangle$ ,  $\langle\mathbf{p}_k\rangle$  and  $\sigma_k^2$  are derived using the time-dependent variational principle (see e.g. [5]) based on the action minimization. For this purpose, we define the action as:

$$S = \int_{t_1}^{t_2} L(\Phi, \Phi^*) dt \quad (17)$$

with the Lagrange functional given as:

$$L = \left\langle \Phi \left| i\hbar \frac{d}{dt} - H \right| \Phi \right\rangle = \left\langle \Phi \left| i\hbar \frac{d}{dt} \right| \Phi \right\rangle - \langle \Phi | H | \Phi \rangle \quad (18)$$

Now we will concentrate on the determination of average value of the Hamiltonian  $\langle \Phi | H | \Phi \rangle$ . As usual the Hamiltonian can be written as the sum of the kinetic energy  $T$  and potential interaction  $V$ . To determine the average kinetic energy we assume that each wave packet has a momentum dispersion  $\sigma_{p_k}$  around its mean value  $\langle \mathbf{p}_k \rangle$ . Then the average kinetic energy associated with the system:

$$\langle \Phi | T | \Phi \rangle = \sum_{k=1}^{k=M} \left[ \frac{\langle \mathbf{p}_k \rangle^2}{2m} + \frac{3\sigma_{p_k}^2}{2m} \right] \quad (19)$$

We assume also that the interaction between nucleons can be described by the potential given in form:

$$V(\{\mathbf{r}_k\}) = V_N(\{\mathbf{r}_k\}) + V_S(\{\mathbf{r}_k\}) + V_{Coul}(\{\mathbf{r}_k\}) \quad (20)$$

where  $V_N$  describes the nuclear interaction,  $V_S$  describes the modification of the interaction induced by changing the density of matter around the nucleon (surface energy) and  $V_{Coul}$  consists of the Coulomb interaction. If the nuclear matter is characterized by non zero spin polarization then, in the space a magnetic field can occur. This field can also be generated by the movement of protons. In such a case the Hamiltonian should be corrected for the magnetic interaction.

Now the average value of the Hamiltonian can be expressed by:

$$\begin{aligned} \langle \Phi | H | \Phi \rangle &= \sum_{k=1}^{k=M} \left[ \frac{\langle \mathbf{p}_k \rangle^2}{2m} + \frac{3\sigma_{p_k}^2}{2m} \right] + \\ &\langle \Phi | V_N | \Phi \rangle + \langle \Phi | V_S | \Phi \rangle + \langle \Phi | V_{Coul} | \Phi \rangle + \langle \Phi | M | \Phi \rangle \end{aligned} \quad (21)$$

In our further considerations we ignore magnetic interaction. The crucial assumption of the present approach is that energy of the fermionic internal motion

can be described by  $\frac{3\sigma_{p_k}^2}{2m}$ , so the sum

$$B_V = \sum_{k=1}^{k=M} \frac{3\sigma_{p_k}^2}{2m} + \langle \Phi | V_N | \Phi \rangle = \int e(\rho, \delta, \sigma_n, \sigma_p) \rho(\mathbf{r}) d^3\mathbf{r} \quad (22)$$

can be treated as a volume term of binding energy. As we know, the ground state energy of nuclear matter is described by the EOS, which considers the energy density as the sum of kinetic energy, associated with the internal fermionic motion, and energy given by the potential interactions. Therefore in our approach we do not have to deal with finding the appropriate distribution of the nucleon momenta, provided that a correct description is given by the selection of appropriate EOS parameters. Such an EOS parameterization replaces the potential parameterization normally used in such approaches.

As in [3], the surface energy is defined as

$$B_{surf} = \langle \Phi | V_S | \Phi \rangle = s_0 \sum_{i=1}^{i=M} \frac{\sigma_e(i)}{\sigma_i^2} \quad (23)$$

where in this semiempirical part  $s_0$  is the surface energy coefficient. In this formula, the variance  $\sigma_e(k)$  denotes the variance of energy  $e(\rho, \delta, \eta_n, \eta_p)$  with respect to the probability  ${}^k\rho(\mathbf{r})$  of finding the  $k$ -th nucleon:

$$\sigma_e(k) = \left[ \int (\bar{e} - e(\rho, \delta, \eta_n, \eta_p))^2 \cdot {}^k\rho(\mathbf{r}) d^3\mathbf{r} \right]^{\frac{1}{2}} \quad (24)$$

where  $\bar{e}$  is the average energy given by the formula:

$$\bar{e}(k) = \int e(\rho, \delta, \eta_n, \eta_p) \cdot {}^k\rho(\mathbf{r}) d^3\mathbf{r} \quad (25)$$

In appendix 1 we describe the method of calculation used for variance  $\sigma_e(k)$  calculations.

Let us discuss briefly the description of the surface energy given by formula (23). In our approach we consider drops of nuclear matter shown in Figure 1. The density of matter  $\rho(r) = \rho_n(r) + \rho_p(r)$  is a function of the distance  $r$  and  $\rho_n(r) = \rho_{n\uparrow} + \rho_{n\downarrow}$  and  $\rho_p(r) = \rho_{p\uparrow} + \rho_{p\downarrow}$ . If the  $l^{th}$  packet is in the region of fixed energy  $e(\rho, \delta, \eta_n, \eta_p)$ , then its variance  $\sigma_e(l)$ , associated with this package  ${}^l\rho(\mathbf{r})$ , is equal to zero. If

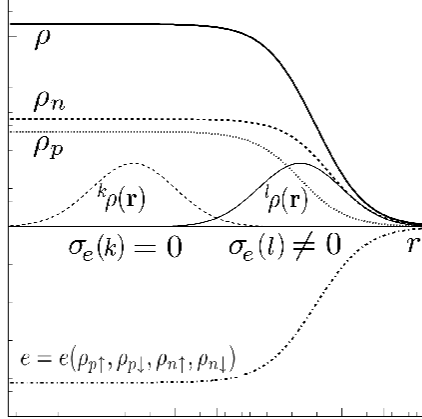


Figure 1: An example of the position of the partial density function and associated energy variance. As one can see for a position close to the center, variance of the energy (24) vanishes. See text for more details.

the package  ${}^k\rho(\mathbf{r})$  is in the change of the energy, then the variance  $\sigma_e(k)$  is greater than zero. According to formula (23), the surface energy associated with the  $i^{th}$  packet is inversely proportional to the uncertainty of location, which means that it is proportional to the indeterminacy of the package momentum. Now formula (23) can be understood as follows. Variation of energy  $\sigma_e(i)$  (and associated forces) describes the possibility of localization of the  $i^{th}$ -th nucleon in case of its entering the alternating field. Such localization forces result in an increase of indeterminacy of the momentum and an increase of the average kinetic energy associated with the  $i^{th}$  package.

The last term in (20) is the Coulomb energy (for protons only) and is given in the form:

$$\langle \Phi | V_{Coul} | \Phi \rangle = \frac{1}{2} \sum_{k \neq l} \int {}^k\rho(\mathbf{r}) \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} {}^l\rho(\mathbf{r}') d^3\mathbf{r} d^3\mathbf{r}' \quad (26)$$

This integral can be calculated analytically as (see eg. [6]):

$$e^2 \sum_{k \neq l} \frac{\text{erf}\left(\frac{r_{kl}}{\sqrt{2}\sigma}\right)}{r_{kl}} \quad (27)$$

where  $r_{kl} = |\langle \mathbf{r}_k \rangle - \langle \mathbf{r}_l \rangle|$  and sigma  $\sigma = \sqrt{\sigma_k^2 + \sigma_l^2}$ .

Finally, the expected form of the Hamiltonian can be written in a form which is analogous to the description given by the liquid drop model (LDM):

$$\langle \Phi | H | \Phi \rangle = \sum_{k=1}^{k=M} \frac{\langle \mathbf{p}_k \rangle^2}{2m} + B_V(\{\langle \mathbf{r}_k \rangle\}, \{\sigma_k\}) + B_S(\{\langle \mathbf{r}_k \rangle\}, \{\sigma_k\}) + V_{Coul}(\{\langle \mathbf{r}_k \rangle\}, \{\sigma_k\}) \quad (28)$$

Based on the Euler-Lagrange equations one can find the corresponding equations of motion for coordinates

$\langle \mathbf{p}_k \rangle$ ,  $\langle \mathbf{r}_k \rangle$  and  $\sigma_k$  [see Euler-Lagrange equations]. This will be described in a forthcoming paper.

Here, as the first test of the new form of the equation of state, based on the MLDM model, we will try to describe the ground state properties of a selected set of nuclei. In our very preliminary approach we will focus on binding energies and nuclear charge radii (RMS).

## 4 The MLDM calculations for describing the ground state properties of nuclei

In the MLDM model the ground state of a nucleus is a many-body state which is an absolute minimum with respect to variation of  $\langle \mathbf{r}_k \rangle$ ,  $\sigma_k$ . Additionally, in the ground state, for every  $k$  the average momentum  $\langle p_k \rangle = 0$ , which means that for MLDM the particle will be essentially at rest and the system corresponds to a solid. In order to determine the nuclear ground state wave function the following procedure of searching the set  $\{\langle \mathbf{r}_k \rangle, \sigma_k\}$  is used:

1. In a limited space we choose a random position of the wave packet together with a certain initial variance. In order to accelerate the calculations, for even-even nuclei, we can also assume a correlation (mating) for packets describing the nucleons of the

same type and differing only in the direction of the spin projection. In such a case we assume that the positions of centers and the variances of a chosen pair are equal.

2. Using a selected set of parameters describing the interaction (type EOS) we search to find such values of these parameters for which the energy of the system is minimal. Here, a variety of methods may be used. One should also be careful to avoid emerging local minima. Wave functions found in this way are characterized by certain symmetries, which may be helpful in assessing the resulting minimum. In the next chapter we will discuss types of symmetry, emerging especially for even-even nuclei with an equal numbers of protons and neutrons.

To use the presented model for calculation of ground state properties of nuclei, we have to select specific values of parameters describing the equation of state. For this purpose a global search for optimal parameters values should be used. This will be done in the next paper, here we apply only a very simplified search method based on following assumptions:

In the first step we try to determine the  $\rho_0$ ,  $e_{00}$ ,  $K_0$  and  $s_0$  parameters. In our preliminary estimations, we assume that  $\rho_0 = 0.159 \text{ nucl/fm}^3$  and  $K = 300 \text{ MeV}$ , which have to be in an experimental and theoretical justification. Then we use the binding energies and RMS radii for  $^4\text{He}$  and  $^{12}\text{C}$  nuclei to determine  $e_{00}$  and  $s_0$  by the trial and error method. In this way we obtain  $e_{00} = -12.9 \text{ MeV}$  and  $s_0 = 0.09 \text{ fm}^2$ . For these nuclei, due to the linking of matter in clusters which are equilibrated in spin and isospin coordinates, corrections arising due to the symmetry energies appear to be negligibly small. Note that the obtained parameters  $e_{00}$  and  $s_0$ , differ from standard values (in particular, the typical value of  $e_{00} = -16 \text{ MeV}$ ). This is a result of their assessment for of very light nuclei. In the future it will be necessary to determine these parameters based on a larger database (the set of the energy and radii of the nuclei in their ground states).

In the next step, we use the binding energy and RMS radii of  $^2\text{H}$ ,  $^3\text{H}$ ,  $^3\text{He}$ , to obtain an estimate of the isospin and spin polarization parameters. Our rough estimate gives  $e_{I0} = 30 \text{ MeV}$ ,  $L_I = 123 \text{ MeV}$ ,  $K_I = 500 \text{ MeV}$  for isospin parameters and  $e_{ii0} =$

$65 \text{ MeV}$ ,  $L_{ii} = 300 \text{ MeV}$ ,  $K_{ii} = 300 \text{ MeV}$  for the spin interaction in gas of neutrons (or protons). The mutual spin interaction of protons and neutrons are described by the parameters  $e_{ij0} = -1 \text{ MeV}$ ,  $L_{ij} = 20 \text{ MeV}$ ,  $K_{ij} = 300 \text{ MeV}$ .

With such parameters, the dependence of the energies  $e_0$ ,  $e_I$ ,  $e_{ii}$  and  $e_{ij}$ , on the density are presented in Figure 2.

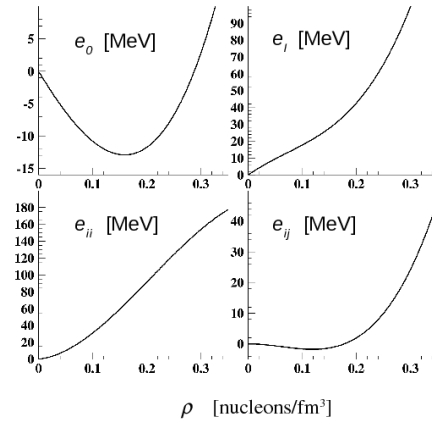


Figure 2: The dependence on the density of nuclear matter:  $e_0$  in an isospin and spin balanced state, the symmetry energy  $e_I$  for isospin of the system, the symmetry energy  $e_{ii}$  for the spin polarization for proton or neutron matter and the symmetry energy  $e_{ij}$  for spin polarization for proton-neutron matter (see text)

In this simple analysis the  $^2\text{H}$ ,  $^3\text{H}$ ,  $^3\text{He}$ ,  $^4\text{He}$  and  $^{12}\text{C}$  nuclei can be treated as generators of the EOS parameters. Reproduced by MLDM model, the binding energy and RMS radii are for this generators arranged together with experimental data in Table 1

For such choice of the EOS parameters (and the coefficient of surface tension  $s_0 = 0.09 \text{ fm}^2$ ) we obtain predictions for the binding energies per nucleon and RMS charge radii these are presented together with experimental data in Table 2.

The data in Table 1 and Table 2 should be treated as very preliminary predictions of the MLDM code

Table 1: MLDM calculation results (for EOS parameters selection, preliminary). Binding energies and RMS charge radii of nuclei are compared with the experimental data.

nuclei	binding energy data (MeV)	binding energy MLDM (MeV)	RMS charge radii data (fm)	RMS charge radii MLDM (fm)
$^2H$	-1.112	-1.104	2.14	2.196
$^3H$	-2.827	-2.809	1.759	1.824
$^3He$	-2.572	-2.571	1.945	1.974
$^4He$	-7.074	-7.062	1.676	1.727
$^{12}C$	-7.68	-7.719	2.47	2.466

Table 2: MLDM calculation results (prediction, preliminary). Binding energies and RMS charge radii of nuclei are compared with the experimental data.

nuclei	binding energy data (MeV)	binding energy MLDM (MeV)	RMS charge radii data (fm)	RMS charge radii MLDM (fm)
$^{16}O$	-7.976	-7.84	2.701	2.613
$^{20}Ne$	-8.032	-7.908	3.005	2.774
$^{24}Mg$	-8.261	-7.953	3.056	2.874
$^{32}S$	-8.493	-7.929	3.261	3.127
$^{36}Ar$	-8.520	-7.896	3.39	3.227
$^{20}Ca$	-8.551	-7.85	3.476	3.336

based on a roughly chosen equation of state. For heavier nuclei one can see quite large deviations from experimental data. In order to achieve greater consistency with the description of experimental data, all EOS parameters need to be re-adjusted.

## 5 The alpha structure of even-even nuclei with equal numbers of protons and neutrons

The concept of nuclear clusters appeared along with the quantum description of nuclei (and even before the discovery of the neutron in 1932 by James Chadwick). In article [7] many experimental arguments are presented for the possible emergence of clusters

of alpha, as a matter substructures in forming nuclei. We present here only two of them, both taken from [8].

i) The binding energy of even-even nuclei with an equal number of protons and neutrons appears to be a linear function of the number of bonds in alpha-particle model, where the number of bonds is equal to:  $k = 1$  for  $^8Be$ ,  $k = 3$  for  $^{12}C$ ,  $k = 6$  to  $^{16}O$ , for  $k = 9$   $^{20}Ne$ , etc. (see Fig. 9). In the cited work this phenomenon is explained on the basis of the proposed form of the potential interaction between the alpha particles, however there is no justification for the increase in the number of bounds, with an increasing number of alpha particles.

ii) The binding energy of nuclei with an even number of protons  $Z$  and an odd, higher by 1 number of neutrons  $N = Z + 1$ . In this case we assume that the excess neutron is interacting with multi-centrist potential defined by the system of the appearing alpha particles. Let the binding energy for each nuclide  $X$  be defined by the function  $b(X)$ . If the neutron binding energy in  $^5He$  is denoted by  $B$ , then we get the following scheme:

$$b(^5He) - [b(^4He) + b(n)] = B$$

$$b(^9Be) - [b(^8Be) + b(n)] = B + (R + Q)$$

$$b(^{13}C) - [b(^{12}C) + b(n)] = B + 2(R + Q)$$

$$b(^{17}O) - [b(^{16}O) + b(n)] = B + 3(R + Q) \quad (29)$$

where the constants  $R$  and  $Q$  are the result of reasoning, which below is presented in the case of  $^9Be$ . If a  $|\psi_1\rangle$  and  $|\psi_2\rangle$  denote the neutron wave functions corresponding to the interaction with the given alpha particle, then the two-centre wave function for  $^8Be$  can be expressed approximately as a linear combination of the single center ones ( $|\psi_1\rangle$  and  $|\psi_2\rangle$ ). Now, the average binding energy of a neutron, in two-centre potential, can be expressed as:



$$b(^9\text{Be}) - [b(^8\text{Be}) + b(n)] = \frac{\langle \psi_1 + \psi_2 | T + V_1 + V_2 | \psi_1 + \psi_2 \rangle}{\langle \psi_1 + \psi_2 | \psi_1 + \psi_2 \rangle} \quad (30)$$

where in the Hamiltonians  $H = T + V_1 + V_2$  operator  $T$  describes the kinetic energy and the  $V_1$  and  $V_2$  are related the neutron interaction with the corresponding alpha particle. As can be seen, the following expressions occur twice in the numerator:

$\langle \psi_1 | T + V_1 | \psi_1 \rangle = B$ , which is the neutron binding energy in  $^5\text{He}$ , and

$\langle \psi_1 | V_2 | \psi_1 \rangle = R$ , which describes the additional energy associated with the presence of the second alpha particle, and

$\langle \psi_1 | H | \psi_2 \rangle = Q$  as the energy associated with the exchange process.

If the wave functions  $|\psi_1\rangle$  and  $|\psi_2\rangle$  are normalized, then the denominator in (30) is equal to  $2(1 + \langle \psi_1 | \psi_2 \rangle)$ . Usually, it can be assumed that  $\langle \psi_1 | \psi_2 \rangle = S$  is of little value compared to 1, and therefore (30) tends to the corresponding part of the expression (29).

These examples show that the nuclear matter in the nuclei has a structure in which the alpha particles seem to play an important role.

The report [7] describes also some of alpha cluster models. Our approach is based on single nucleons and in this way it is similar to QMD (Quantum Molecular Dynamics) [9], AMD (Antisymmetrized Molecular Dynamics) [10] and FMD (Fermionic Molecular Dynamics) [11], in which the dynamics description is based on variational principle.

Since our model includes isospin and spin interactions occurring between different types of nucleons with densities  $\rho_{p\uparrow}, \rho_{p\downarrow}, \rho_{n\uparrow}, \rho_{n\downarrow}$ , nucleons are grouped in order to minimize this additional energy. As we know, in the case of fermions this causes the connection of particles into pairs. For nuclear matter an additional positive energy is associated with the lack of isospin balance. To minimize both of these energies, nucleons create alpha clusters. This phenomenon is included in our model, so one can observe the alpha structure in the resulting nuclear matter distribution, particularly for even-even nuclei with equal proton and neutron numbers. To show this we present in

Fig 3-6 the results of calculations for the nuclei  $^{16}\text{O}$ ,  $^{24}\text{Mg}$ ,  $^{36}\text{Ar}$  and  $^{40}\text{Ca}$ .

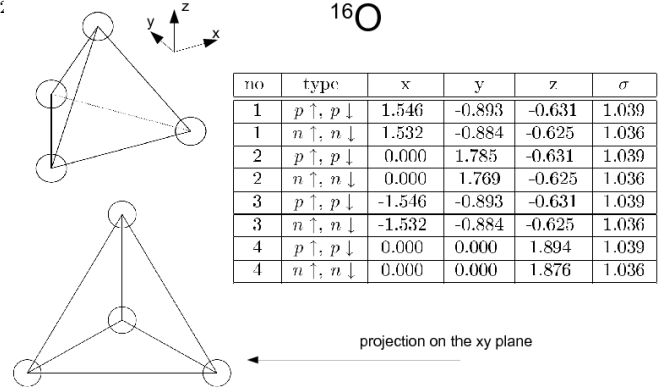


Figure 3: The position and the variance of the wave packet for the nucleons in the nucleus  $^{16}\text{O}$ . In the first column of the table contained in the figure there are the numbers of groups of nucleons, which are correlated in the alpha particle. The second column indicates the spins and type of nucleons creating given pairs of nucleons. The common position and variance of the two wave packets is presented.

The alpha structures obtained in our calculations are identical with the structures presented in papers [8], [12] up to the silicon and the number of alpha-alpha bonds are the same as that proposed by [13] (after  $^{16}\text{O}$  there is an increment of three bonds for each additional alpha particle). Thus we have 15 bonds for  $^{28}\text{Si}$  instead of 16 [8]. The justification (but that need not be the final) for this selection can be understood from Fig. 7 for alpha-alpha distance distribution.

This distribution shows that the countable alpha-alpha bond distances are centered around 3.23 fm up to 3.5 fm. In the case of  $^{28}\text{Si}$ , the distances associated with 15 bonds lie below this value and the rest has distances greater than 4.0 fm. In our model calculation, a systematic increase in the binding energy can be observed up to  $^{56}\text{Ni}$ . In this range ( $2 \leq Z \leq 28$ ),

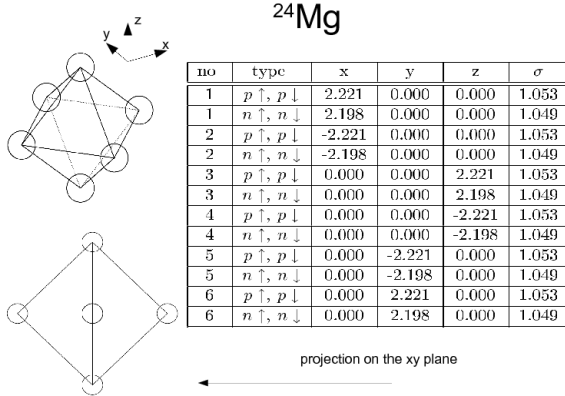


Figure 4: The position and the variance of the wave packet for the nucleons in the nucleus  $^{24}\text{Mg}$ . Notation is the same as in Figure 3.

systematics follows Bethe's prediction [13], and the resulting geometrical arrangement of alpha particle has a "balloon structure" (no alpha particles present inside the structure). The model results also indicate that the first (lightest) nucleus for which the alpha particle appears inside the structure is  $^{60}\text{Zn}$  (see Fig 8). This results in a departure from the systematic increase in energy presented in the Fig 9.

## 6 Conclusions

A new form of the EOS suitable for the MLDM model calculations is presented. Preliminary results show that the MLDM model is able to reproduce the basic properties of atomic nuclei. We see also that MLDM fairly well describes the properties of very light nuclei. Because these particles are usually manufactured with the highest probability this is important for a correct description of the reaction dynamics.

Another important property of the model, resulting from taking into account the mutual interaction related to the spin and isospin of nucleons, is the emergence of the alpha structures which is particularly noticeable for even-even nuclei with equal numbers of protons and neutrons. This formation of alpha

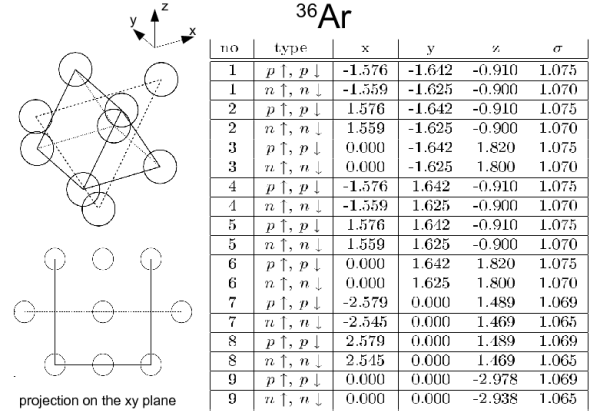


Figure 5: The position and the variance of the wave packet for the nucleons in the nucleus  $^{36}\text{Ar}$ . Notation is the same as in Figure 3.

clusters is in line with the considerations on the binding energy gain associated with the resulting increase in the number of bonds between alpha particles. It seems that the model can be helpful in determination of the number of bonds. An important prediction of the model and strong support for the hypothesis of alpha clusters is the appearance of alpha particles inside surface structure for the  $Z > 28th$ . This creates an additional branch in the scheme of the binding energy growth as can be seen in the experimental systematics. A detailed analysis of the binding energy (as energy per nucleon) for the cases discussed above show that there are some additional effects. This shows that the number of alpha bonds may differ slightly in each individual case. The analysis of this behavior as well as restrictions on the applicability of the present simple model will be presented in forthcoming paper.

We need to emphasize the very preliminary character of these results. In order to better predict the values of the EOS parameters further work is needed and we have to perform a global search in which we will take into account all available experimental data. It would also help to compare the model results, describing the basic observables for heavy ion reactions (particularly for the compressibility factor  $K_0$ ) in the

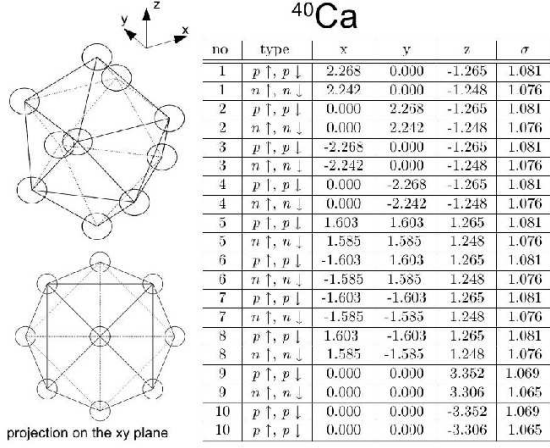


Figure 6: The position and the variance of the wave packet for the nucleons in the nucleus  $^{40}\text{Ca}$ . Notation is the same as in Figure 3.

low energy region where the impact of the nucleon-nucleon collisions can be neglected.

## acknowledgement

The authors are indebted to Professor L. Jarczyk and Professor R. Planeta for reading the manuscript and a fruitful discussion.

This work was supported in part by the Foundation for Polish Science MPD program, co-financed by the European Union within the European Regional Development Fund.

This work was supported also by the IN2P3 grant number 08-128.

## Appendix A

In this appendix, it is derived the form of EOS which is used in the paper. We start from the expansion of the energy density function and we use the symmetry which exists in nuclear interactions. According to this symmetry, in the expansion (up to 4 order) of the  $e(\xi, \delta, \eta_n, \eta_p)$  around the point:  $\xi = 0, \delta = 0, \eta_n =$

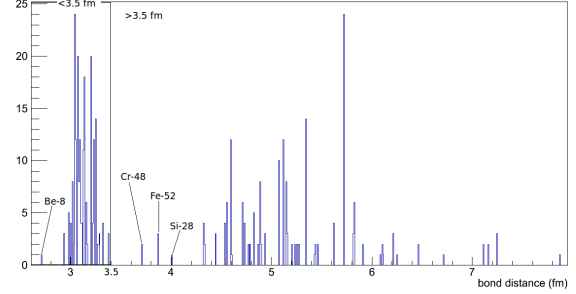


Figure 7: The distribution alpha-alpha interparticle distance calculated with MLDM is plotted (up to  $^{56}\text{Ni}$ ). Most of the countable distance lies below 3.5 fm (not a final conclusion). For  $^{28}\text{Si}$ ,  $16^{\text{th}}$  bond length is shown.

0,  $\eta_p = 0$  only the following terms can appear:

$$e = e_0 + \frac{1}{2}e_{\xi\xi}\xi^2 +$$

$$\delta^2 \left( \frac{1}{2}e_{\delta\delta} + \frac{1}{4}e_{\delta\delta S_n S_n}\eta_n^2 + \frac{1}{2}e_{\delta\delta S_n S_p}\eta_n\eta_p + \frac{1}{4}e_{\delta\delta S_p S_p}\eta_p^2 + \frac{1}{2}e_{\xi\delta\delta\xi} + \frac{1}{4}e_{\xi\xi\delta\delta\xi^2} \right) +$$

$$\eta_n^2 \left( \frac{1}{2}e_{\eta_n\eta_n} + \frac{1}{24}e_{\eta_n\eta_n\eta_n\eta_n}\eta_n^2 + \frac{1}{4}e_{\eta_n\eta_n\eta_p\eta_p}\eta_p^2 + \frac{1}{2}e_{\xi\eta_n\eta_n}\xi + \frac{1}{4}e_{\xi\xi\eta_n\eta_n}\xi^2 \right) +$$

$$\eta_p^2 \left( \frac{1}{2}e_{\eta_p\eta_p} + \frac{1}{24}e_{\eta_p\eta_p\eta_p\eta_p}\eta_p^2 + \frac{1}{2}e_{\xi\eta_p\eta_p}\xi + \frac{1}{4}e_{\xi\xi\eta_p\eta_p}\xi^2 \right) +$$

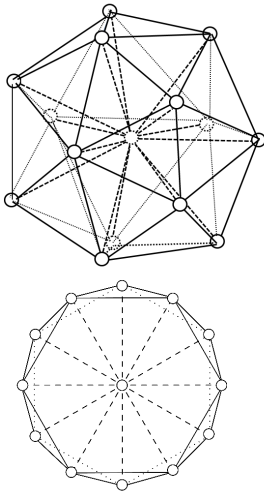
$$\eta_n\eta_p \left( e_{\eta_n\eta_p} + e_{\xi\eta_n\eta_p}\xi + \frac{1}{2}e_{\xi\xi\eta_n\eta_p}\xi^2 \right) \quad (31)$$

The symbol  $e$  with the index constituting one of the variables of the equation denotes a derivative of the energy density with respect to this variable. We neglect the dependence on  $\delta^4$  and for small spin polarization the terms in the brackets containing  $\eta_n^2, \eta_p^2, \eta_n\eta_p$  can be neglected in relation to  $e_{\delta\delta}, e_{\eta_n\eta_n}, e_{\eta_p\eta_p}$ , and finally one can write:

$$e = e_0 + \frac{1}{2}e_{\xi\xi}\xi^2 +$$

$$\delta^2 \left( \frac{1}{2}e_{\delta\delta} + \frac{1}{2}e_{\xi\delta\delta\xi} + \frac{1}{4}e_{\xi\xi\delta\delta\xi^2} \right) +$$

$$\eta_n^2 \left( \frac{1}{2}e_{\eta_n\eta_n} + \frac{1}{2}e_{\xi\eta_n\eta_n}\xi + \frac{1}{4}e_{\xi\xi\eta_n\eta_n}\xi^2 \right) +$$



No:	Type	x	y	z	$\sigma$
1	$p \uparrow p \downarrow$	0.000	0.000	0.000	1.184
1	$n \uparrow n \downarrow$	0.000	0.000	0.000	1.165
2	$p \uparrow p \downarrow$	1.704	-1.959	-1.506	1.082
2	$n \uparrow n \downarrow$	1.681	-1.933	-1.485	1.074
3	$p \uparrow p \downarrow$	-2.246	-1.375	2.148	1.082
3	$n \uparrow n \downarrow$	-2.215	-1.356	2.118	1.076
4	$p \uparrow p \downarrow$	1.009	1.018	-3.081	1.082
4	$n \uparrow n \downarrow$	0.995	1.003	-3.038	1.076
5	$p \uparrow p \downarrow$	-3.348	-0.293	-0.507	1.082
5	$n \uparrow n \downarrow$	-3.301	-0.289	-0.500	1.076
6	$p \uparrow p \downarrow$	3.102	1.110	-0.834	1.082
6	$n \uparrow n \downarrow$	3.058	1.094	-0.822	1.076
7	$p \uparrow p \downarrow$	0.276	-0.133	3.385	1.082
7	$n \uparrow n \downarrow$	0.272	-0.131	3.337	1.076
8	$p \uparrow p \downarrow$	0.641	-2.917	1.622	1.082
8	$n \uparrow n \downarrow$	0.632	-2.876	1.599	1.076
9	$p \uparrow p \downarrow$	-1.266	-1.041	-2.977	1.082
9	$n \uparrow n \downarrow$	-1.248	-1.027	-2.935	1.076
10	$p \uparrow p \downarrow$	-1.451	-3.009	-0.625	1.082
10	$n \uparrow n \downarrow$	-1.430	-2.967	-0.616	1.076
11	$p \uparrow p \downarrow$	0.595	3.274	-0.688	1.082
11	$n \uparrow n \downarrow$	0.586	3.229	-0.679	1.076
12	$p \uparrow p \downarrow$	-1.704	1.959	1.506	1.081
12	$n \uparrow n \downarrow$	-1.681	1.933	1.485	1.074
13	$p \uparrow p \downarrow$	1.696	2.192	1.966	1.082
13	$n \uparrow n \downarrow$	1.673	2.161	1.939	1.076
14	$p \uparrow p \downarrow$	2.918	-0.857	1.517	1.082
14	$n \uparrow n \downarrow$	2.877	-0.845	1.496	1.076
15	$p \uparrow p \downarrow$	-1.927	2.032	-1.926	1.082
15	$n \uparrow n \downarrow$	-1.900	2.003	-1.898	1.076

Figure 8: The alpha particle structure of  $^{60}\text{Zn}$  obtained via MLDM calculation. Noticeable thing is that there is an alpha particle inside the balloon like structure (the structural change starts from here, see the text for detail).

$$\eta_p^2 \left( \frac{1}{2} e_{\eta_p \eta_p} + \frac{1}{2} e_{\xi \eta_p \eta_p} \xi + \frac{1}{4} e_{\xi \xi \eta_p \eta_p} \xi^2 \right) + 2\eta_n \eta_p \left( \frac{1}{2} e_{\eta_n \eta_p} + \frac{1}{2} e_{\xi \eta_n \eta_p} \xi + \frac{1}{4} e_{\xi \xi \eta_n \eta_p} \xi^2 \right) \quad (32)$$

Replacing symbols of derivatives  $e_{\lambda \dots}$  by variables defined in the following relations:

$$\begin{aligned} \frac{K_0}{18} &= \frac{1}{2} e_{\xi \xi} \\ e_{I0} &= \frac{1}{2} e_{\delta \delta}, \quad \frac{L_I}{3} = \frac{1}{2} e_{\xi \delta \delta}, \quad \frac{K_I}{18} = \frac{1}{4} e_{\xi \xi \delta \delta} \\ e_{ii0} &= \frac{1}{2} e_{\eta_n \eta_n}, \quad \frac{L_{ii}}{3} = \frac{1}{2} e_{\xi \eta_n \eta_n}, \quad \frac{K_{ii}}{18} = \frac{1}{4} e_{\xi \xi \eta_n \eta_n} \\ e_{ij0} &= \frac{1}{2} e_{\eta_n \eta_p}, \quad \frac{L_{ij}}{3} = \frac{1}{2} e_{\xi \eta_n \eta_p}, \quad \frac{K_{ij}}{18} = \frac{1}{4} e_{\xi \xi \eta_n \eta_p} \end{aligned} \quad (33)$$

and taking into account the mentioned symmetries of nuclear interactions (the derivatives  $(e_{\eta_p \eta_p}, e_{\eta_n \eta_n})$ ,

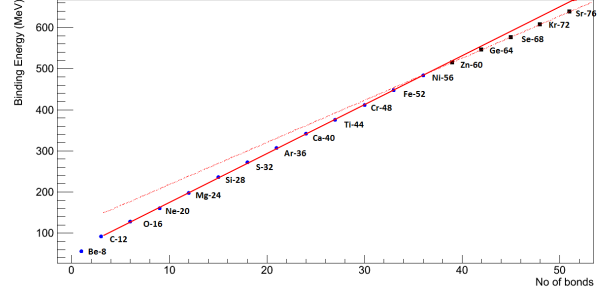


Figure 9: Total binding energy of the nuclei versus number of bonds. From  $^{12}\text{C}$  to  $^{56}\text{Ni}$ , it follows the same linear relationship, according to surface-like structures. From  $^{60}\text{Zn}$ , slope has a new linear relationship reflecting change occurring in the nuclei structures, (see text for detail).

$(e_{\xi \eta_p \eta_p}, e_{\xi \eta_n \eta_n})$  and  $(e_{\xi \xi \eta_p \eta_p}, e_{\xi \xi \eta_n \eta_n})$  are pairwise equal, this means that the respective symmetry energy associated with the spin is identical for protons and neutrons), we obtain the equation (7).

## Appendix B

In this appendix we present the method of calculation of the variance of energy given by the EOS in the neighborhood of the center of the packet  $k$ . In the first step we calculate the average energy density of matter at random points with the distribution of  $^k \rho(\mathbf{r})$ .

$$\bar{e}(k) = \int e(\rho, \delta, \eta_n, \eta_p) \cdot ^k \rho(\mathbf{r}) d^3 \mathbf{r} \quad (34)$$

If we use the equation of state in the form of an expansion (7) and (11) for the isospin part the derived term cannot be solved analytically:

$$\begin{aligned} \int \delta^2 \alpha_I \rho \cdot ^k \rho(\mathbf{r}) d^3 r &= \alpha_I \int \left( \frac{\rho_n - \rho_p}{\rho} \right)^2 \rho \cdot ^k \rho(\mathbf{r}) d^3 r \\ &= \alpha_I \int \frac{\rho_n \rho_n - 2\rho_n \rho_p + \rho_p \rho_p}{\rho} \cdot ^k \rho(\mathbf{r}) d^3 r \end{aligned} \quad (35)$$

In order to avoid this problem we can use the following approximations:

$$\alpha_I \int \frac{\rho_n \rho_n}{\rho} \cdot^k \rho(\mathbf{r}) d^3 \mathbf{r} \cong \alpha_I \frac{N}{A} \int \rho_n \cdot^k \rho(\mathbf{r}) d^3 \mathbf{r} \quad (36)$$

where  $N$  and  $A$  are the total number of neutrons and nuclei in the system, respectively. As we can see, after removing  $\rho$  from the denominator the integral can be solved analytically. Similarly, we can find the remaining ingredients (35) (with  $\rho_n \rho_p$  and  $\rho_p \rho_p$ ).

In the next step we assume that the  $\delta$ ,  $\eta_n$ ,  $\eta_p$  are established in the vicinity of the nucleon  $k$  as  $\bar{\delta}(k)$ ,  $\bar{\eta}_n(k)$ ,  $\bar{\eta}_p(k)$  (we replace them by the corresponding average values) and we determine the effective density of  $\rho_{ef}(k)$  based on the equation:

$$\bar{e}(k) = e(\rho_{ef}(k), \bar{\delta}(k), \bar{\eta}_n(k), \bar{\eta}_p(k)) \quad (37)$$

In further considerations we replace the set

$\rho_{ef}(k)$ ,  $\bar{\delta}(k)$ ,  $\bar{\eta}_n(k)$ ,  $\bar{\eta}_p(k)$  by  $\tilde{\rho}_{p\uparrow}(k)$ ,  $\tilde{\rho}_{p\downarrow}$ ,  $\tilde{\rho}_{n\uparrow}(k)$ ,  $\tilde{\rho}_{n\downarrow}(k)$ . To calculate the variance  $\sigma_e^2(k)$  we develop the integral expression:

$$\sigma_e^2(k) = \int (\bar{e} - e(\rho_{p\uparrow}, \rho_{p\downarrow}, \rho_{n\uparrow}, \rho_{n\downarrow}))^2 \cdot^k \rho(\mathbf{r}) d^3 \mathbf{r} \quad (38)$$

around  $\tilde{\rho}_{p\uparrow}(k)$ ,  $\tilde{\rho}_{p\downarrow}$ ,  $\tilde{\rho}_{n\uparrow}(k)$ ,  $\tilde{\rho}_{n\downarrow}(k)$ . This allows the analytical calculation of the the considered integral. In our calculations we limited ourselves to the first of order expansion. So, because  $e(\tilde{\rho}_{p\uparrow}(k), \tilde{\rho}_{p\downarrow}(k), \tilde{\rho}_{n\uparrow}(k), \tilde{\rho}_{n\downarrow}(k)) = \bar{e}(k)$  this choice of expansion gives a very simple form of the integrand.

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